Structure and Dynamics in Boron- and Fluoride-Containing Oxide Glasses and Liquids: High-Resolution and High-Temperature Nuclear Magnetic Resonance Studies

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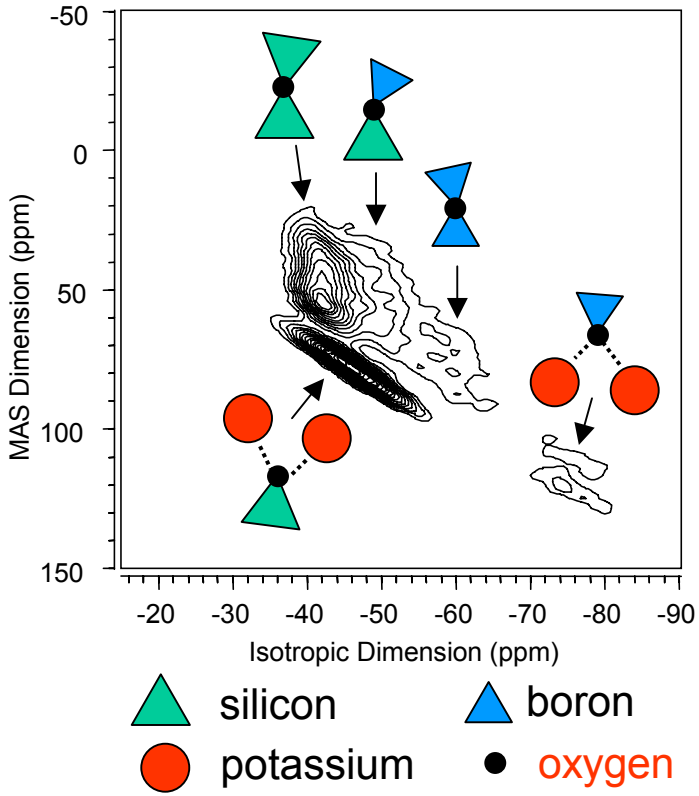
Oxide glasses are widely used by society, with everyday (e.g. beverage containers) to "high-tech" (e.g. optical data processing) applications. Nuclear Magnetic Resonance (NMR) is one of the best methods for measuring the atomic-scale structure of these materials, which is crucial to formulating predictive models of their chemical and physical properties. We are using NMR to "count" the basic structural building blocks of two especially useful types of glasses and glass melts, those containing boron and/or fluoride ions.

J. Non-Cryst. Solids **306**, 160 (2002)
J. Non-Cryst. Solids **315**, 239 (2003)
J. Phys. Chem. B, **107**, 10063 (2003)
Chem. Material. **15**, 3913 (2003)



Oxygen-17 "3QMAS" NMR spectrum of a potassium borosilicate glass. Contour heights reveal percentages of oxygen atoms linking different metal ions in the structure.

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Education:

One Ph.D. student (T.J. Kiczenski) and one postdoctoral student (Lin-Shu Du) are currently supported by this grant. The research is an integral part of their training and career development. We are also developing course materials, based on this project, to educate materials and earth scientists in the fundamentals of structural order/disorder and their role in thermodynamic and transport properties. For example, the two, 2-D analogs of borosilicate networks (shown at right) have very different energetics because of their different proportions of "like" vs. "unlike" linkages.